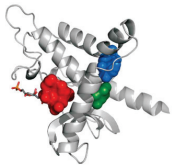
INTELLIGENTPHARMA

Developing solutions. Discovering drugs.

Intelligent Pharma offers different services in computer aided drug discovery. Our molecular modeling department carries out research projects to help your team design and develop new drugs using our computational chemistry expertise.

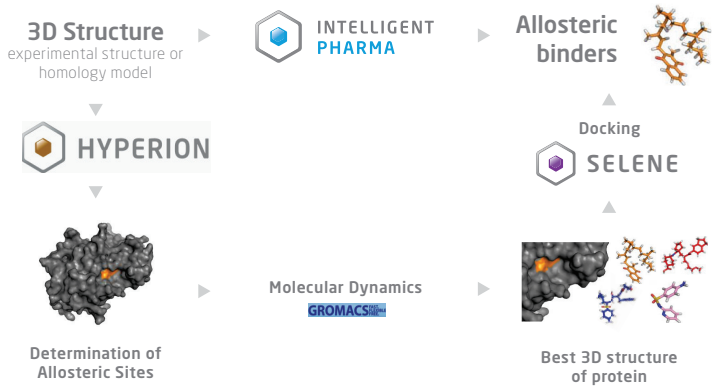
ALLOSTERIC SITES

Allosteric Sites on protein surfaces are good drug targets as they can change the protein's activity and function through manipulating the protein's conformation.

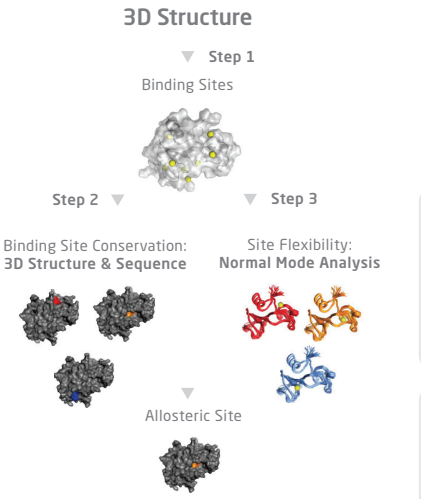


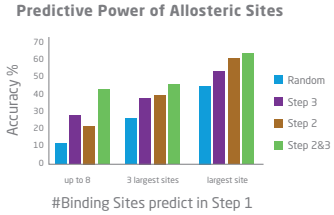
Allosteric site with regulator (red), Active site (blue & green)

DETERMINATION OF ALLOSTERIC LIGANDS



HYPERION





CASE STUDY

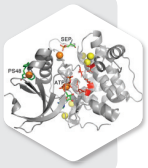
Predicted Binding Sites are shown as Spheres:

Allosteric site

Other binding sites

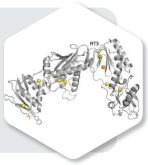
PDK1 kinase

The largest pocket matches the binding site of ATP. The second largest predicted pocket matches the location of the allosteric activator PS48. Another predicted pocket matches the position of a phosphoserine (SEP) in the activation loop of PDK1.



L-lactate dehydrogenase

The two significant pockets match a 'hinge-like' position between different domains, a good position for allosteric ligands



Glyceraldehyde 3-phosphate dehydrogenase

The fifth largest predicted pocket matches the location of the allosteric effector F6P. When a ligand occupying this pocket is simulated, the overall flexibility of the protein is significantly affected on all ranges including the lowest frequency modes.